CONSTITUTIVE LAWS FOR METALLIC INTERFACE SEPARATION MOTIVATED BY NANOSCALE SIMULATIONS

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By incorporating nanoscale fracture dependencies derived from molecular dynamics (MD) simulations using embedded-atom method (EAM) potentials [1], a framework is developed to characterize fracture through continuum interface separation constitutive laws that are motivated by nonlocal atomistic calculations. These laws are distinguished from previous continuum models in that discrete atomistics are used to characterize the nanoscale effects, such as the nature of atomic structure and imperfections on the initiation and propagation of cracks. This conceptual framework utilizes Internal State Variable (ISV) theory [2] to embed a set of interface attributes into cohesive interface separation constitutive relations. An elastic separation potential is developed, with explicit dependence on a set of nanoscale ISVs. Normal and tangential interface displacements are normalized by the set of path-history dependent interface attributes. The proposed list of ISVs accounts for composition, impurities, dislocation density, and nanoporosity within the interface region. Structural rearrangement of the interface region during separation can be explicitly tracked through a set of differential equations for each evolving ISV.

Atomistic calculations will show the evolution of nanoporosity (damage) in the separation process zone for a Cu-Cu interface over a range of non-equilibrium loading paths. Damage within the process zone is measured using a change of coordination number approach. The role of dislocations is highlighted in a series of simulations involving normal and shear interface separations, as well as sequences of normal-shear and shear-normal deformation relative to the interface. A centrosymmetry parameter approach is used to estimate dislocation line length per unit volume in the separation zone. Concepts are outlined for scaling up continuum separation laws that are consistent with regard to dissipation across change of scale and invoke some notion of thermodynamic equivalence to the atomistic calculations [3].

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